

Programming OpenMP

Christian Terboven

Michael Klemm



Agenda (in total 7 Sessions)



Session 1: OpenMP Introduction

- → Welcome
- → OpenMP Overview
- \rightarrow Parallel Region
- → Worksharing
- → Scoping
- \rightarrow Tasking (short introduction)
- → Executing OpenMP programs
- →Homework assignments ☺
- → Compile and run on Perlmutter CPUs
- Session 2: Tasking
- Session 3: Optimization for NUMA and SIMD
- Session 4: What Could Possibly Go Wrong Using OpenMP
- Session 5: Introduction to Offloading with OpenMP
- Session 6: Advanced OpenMP Offloading Topics
- Session 7: Selected / Remaining Topics



Programming OpenMP

An Overview Of OpenMP

Christian Terboven

Michael Klemm





History

- De-facto standard for Shared-Memory Parallelization.
- 1997: OpenMP 1.0 for FORTRAN
- 1998: OpenMP 1.0 for C and C++
- 1999: OpenMP 1.1 for FORTRAN
- 2000: OpenMP 2.0 for FORTRAN
- 2002: OpenMP 2.0 for C and C++
- 2005: OpenMP 2.5 now includes both programming languages.
- 05/2008: OpenMP 3.0
- 07/2011: OpenMP 3.1
- 07/2013: OpenMP 4.0
- 11/2015: OpenMP 4.5
- 11/2018: OpenMP 5.0
- 11/2020: OpenMP 5.1
- 11/2021: OpenMP 5.2

Members of the OpenMP Language Committee



RWTH Aachen University is a member of the OpenMP Architecture Review Board (ARB) since 2006. Main topics: • Affinity

- Tasking
- Tool support
- Accelerator support



What is OpenMP?

- Parallel Region & Worksharing
- Tasking

...

- SIMD / Vectorization
- Accelerator Programming
- Memory Management





What is OpenMP?

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Get your C/C++ and Fortran Reference Guide! Covers all of OpenMP 5.2!

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Getting Started Navigating this reference guide Description of started and started	OpenMP openmp.org	OpenMP 5.2 API Syntax Referen The OpenMP* API is a scalable model that gives parallel programmers a simple and flexible interface for developing portable parallel applications in C/C++ and Fortran. n ontent [n.n.n] Sections in 5.2. spec [n.n.n]	ce Guide OpenMP is suitable for a wide range of algorithms running on multicore nodes and chips, NUMA systems, GPUs, and other suc devices attached to a CPU. Sections in 5.1. spec See Clause info on pg
Avigating this reference guide Density of the second	Getting Started		
Descriptions and Constructs Specify Constructs consists of a directive and, if defined in the syntax, an associated structured block that follows: • OpenAPP directives succept and and any directives may not appear in Fortran APP (procedures, • a syntax representation of a block of directivele structured block that follows: • OpenAPP directives succept and and any directive and specify the fortran APP (procedures, • a syntax representation of a block of directive structured block that follows: • OpenAPP directives succept and and any directive and directive structure directive and syntax is a longer and any directive structure direc	Navigating this reference guide Droths and Cranual	OpenMP directive syntax A directive is a consistion of the base-language methnism and a stretcive-periodization the directive- name followed by aptroal clause; A construct consists of a forective and the additional base integrate code code. Centers an formed exclusionly with pagents. The constructive and the constructive and the additional formed forective and the constructive and the construction formed forective and the constructive and the construction formed form sources (codes).	Complex: (C+ Byragma amp directive specification (Ilgoing materialed (interfield) (interfield) Ilgoing materialed (interfield) Ilgoing materialed (interfield) Ilgoing materialed (interfield) Ilgoing materialed
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Directives and Constructs (continued) declare simd [7.7] [2.11.5.3] begin]declare variant [7.5.4-5] [2.3.5] clares a specialized variant of a base function and the ntext in which it is used. Applied to a function or subroutine to enable creation of one or more versions to process multiple arguments using SIMD instructions from a single invocation in a SIMD loop Foragma omp declare variant/variant-func-id) Apragma omp declare simd [clouse] [,]clouse] ...] [Vpragma cmp declare variant[variant-func-id] \ clouse [] [,] clouse] ...] (Apragma omp declare simd (clouse(/, clouse) ...)) function definition or declaration - JJ function definition or declaration Somp declare simd /(proc-name)/ Idouse/ [.idouse] ... [Ppragma omp begin declare variant clouse-motch **Ppragma omp end declare variant** aligned (orgument-list) : alignmentil ISomp declare variant (/bose-proc-name : / & variant-proc-name) clause // (,) clause/ / Declares one or more list items to be aligned to the specified number of bytes. alignment: Optional constant positive integer adjust_args (adjust-op : argument-list) expression adjust-on: nothing, need device ptr inbranch linear (linear-list)': linear-step)) append_args (oppend-op/[, oppend-op] ...]} aspend-on: interon (interop-type [[, interop-type] ...]) Specifies the preferred number of iterations to enter be executed concurrently. uniform (argsment-list) match (context-selector-specification) REQUIRED. Specifies how to adjust the arguments of the base function when a specified variant function is selected for replacement. Declares arguments to have an invariant value for all concurrent invocations of the function in the execution of a single SIMD loop. nariant-func-id [begin]declare target [7.8.1-2] [2.14.7] A declarative direction to the set of the set The name of a function variant that is a base larative directive that specifies that variables ons, and subroutines are mapped to a device language identifier, or for C++, a template-id. variant-proc-name Apragma omp declare target (extended-list) The name of a function variant that is a base language identifier. Apragma omp declare target clouse/ [_kclouse ...] se-motch: match (context-selector-specification) Apragma omp begin declare target \ [clause][,[clause]...] declaretions.deficition.com REQUIRED match clause lispatch [7.6] [2.3.6] #pragma omp end declare target witrols whether variant substitution occurs for a function If in the structured block. ISomp declare target (extended-list) #pragma omp dispatch [clouse ([,] clouse] ...] function-dispatch-structured-block !Somp declare target [clouse] [, [clouse] ...] device_type (host | nohost | any) Somp dispatch (clouse [[,] clouse] ...] [Some end dispatch structured block enter (extended-list) A comma-separated list of named variable: procedure names, and named common blocks. depend ((depend-modifier,) dependence-type : locator-list) indirect[(invoked-by-/ptr)] Determines if the procedures in an enter clause device (onto-integer-expression) El may be invoked indirectly. Identifies the target device that is associated link (Ust) with a device construct. Supports compilation of functions called in a is_device_ptr (/ist) target region that refer to the Ast items. list: device pointers · For the second QC++ form of declare target, at least context (omp-logical-expression) If omp-logical-expression evaluates to true, the construct is not added to the construct set of one clause must be enter or link. · For begin declare target, the enter and link clauses the OpenMP context. are not permitted wariants (omp-log/col-expression) If omp-logical-expression evaluates to true, no function variant is selected for the call in the applicable dispatch region. nowait [3] www.openmp.org

OpenMP API 5.2 0/C++ content | Forth

Informational and utility directives requires [8.2] [2.5.1] ecifies the features that an implementation must provid in order for the code to compile and to execute correctly. Apragma omp requires clouse [[[,] clouse] ...] |Somp requires clouse [[[,] clouse] ...] atomic_default_mem_order (seq_cst | acq_rel | relaxed) dynamic_allocators minim_allocators Enables memory allocators to be used in a target region without specifying the uses_allocators clause on the corresponding target construct. [See target on page 5 of this guide.] reverse offload Requires an implementation to guarantee that if a target construct specifies a device clause in which the ancestor modifier appears, the target region can execute on the parent device of an enclosing target region. (See target on page 5.) unified address Requires that all devices accessible through OpenMP API routines and directives use a unified address space. unified_shared_memory Guarantees that in addition to the requir of unified_address, storage locations in memory are accessible to threads on all available devices. assume, [begin]assumes [8.3.24] [2.5.2] Provides invariants to the implementation that may be sed for optimization purposes Apragma omp assumes clouse [[[,] clouse] ...] #pragma omp begin assumes clouse [[[,] clouse] ... , declaration-definition-seq Apragma omp end assumes #pragma omp assume clouse [[[,] clouse]...] ISomp assumes clouse [[[,] clouse] ...] Somp assume clouse [] [,] clouse] ...] ISomp end assume ISomp assume clouse [[[,] clouse] ...] [I\$omp end assume] absent (directive-name (), directive-name) ... It Lists directives absent in the scope. contains (directive-name [], directive-name] ...]] Lists directives likely to be in the scope. holds (onp-logical-expression) An expression guaranteed to be true in the no_openmp Indicates that no OpenMP code is in the scope. no openmp routines Indicates that no OpenMP runtime library calls are executed in the scope. no_parallelism Indicates that no OpenMP tasks or SIMD constructs will be executed in the scope.

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OpenMP Tutorial Members of the OpenMP Language Committee

Recent Books About OpenMP





A printed copy of the 5.2 specifications, 2021



A book that covers all of the OpenMP 4.5 features, 2017



A book about the OpenMP Common Core, 2019



Programming OpenMP

Parallel Region

Christian Terboven

Michael Klemm



OpenMP

OpenMP's machine model

• OpenMP: Shared-Memory Parallel Programming Model.



All processors/cores access a shared main memory.

Real architectures are more complex, as we will see later / as we

Parallelization in OpenMP employs multiple threads.



The OpenMP Memory Model

- All threads have access to the same, globally shared memory
- Data in private memory is only accessible by the thread owning this memory
- No other thread sees the change(s) in private memory
- Data transfer is through shared memory and is 100% transparent to the application





The OpenMP Execution Model

- OpenMP programs start with just one thread: The *Initial Thread*.
- Worker threads are spawned at Parallel Regions, together with the initial thread they form the Team of threads.
- In between Parallel Regions the Worker threads are put to sleep.
 The OpenMP *Runtime* takes care of all thread management work.
- Concept: Fork-Join.
- Allows for an incremental parallelization!





Parallel Region and Structured Blocks

• The parallelism has to be expressed explicitly.

C/C++	Fortran
<pre>#pragma omp parallel</pre>	!\$omp parallel
{	• • •
	structured block
structured block	
•••	!\$omp end parallel
}	

- Structured Block
 - Exactly one entry point at the top
 - Exactly one exit point at the bottom
 - Branching in or out is not allowed
 - Terminating the program is allowed (abort / exit)

- Specification of number of threads:
 - Environment variable: OMP_NUM_THREADS=...
 - Or: Via num_threads clause:
 add num_threads (num) to the parallel construct



Programming OpenMP

Using OpenMP Compilers

Christian Terboven Michael Klemm



Production Compilers w/ OpenMP Support



- GCC
- clang/LLVM
- HPE CPE
- AOCC, AOMP, ROCmCC
- Intel Classic and Next-gen Compilers
- IBM XL
- ... and many more
- See <u>https://www.openmp.org/resources/openmp-compilers-tools/</u> for a list

Compiling OpenMP



- → clang: -fopenmp
- → HPE/Cray CPE: -homp or -fopenmp
- → AOCC, AOCL, ROCmCC: -fopenmp
- → Intel: -fopenmp or -qopenmp (classic) or -fiopenmp (next-gen)

→ IBM XL: -qsmp=omp

Switches have to be passed to both compiler and linker:

```
$ gcc [...] -fopenmp -o matmul.o -c matmul.c
$ gcc [...] -fopenmp -o matmul matmul.o
$./matmul 1024
Sum of matrix (serial): 134217728.000000, wall time 0.413975, speed-up 1.00
Sum of matrix (parallel): 134217728.000000, wall time 0.092162, speed-up 4.49
```



Starting OpenMP Programs on Linux

• From within a shell, global setting of the number of threads:

export OMP_NUM_THREADS=4
./program

• From within a shell, one-time setting of the number of threads:

```
OMP_NUM_THREADS=4 ./program
```





Hello OpenMP World





Programming OpenMP

Worksharing

Christian Terboven

Michael Klemm





For Worksharing

- If only the *parallel* construct is used, each thread executes the Structured Block.
- Program Speedup: *Worksharing*
- OpenMP's most common Worksharing construct: for

C/C++	Fortran
<pre>int i; #pragma omp for for (i = 0; i < 100; i++) { a[i] = b[i] + c[i]; }</pre>	<pre>INTEGER :: i !\$omp do DO i = 0, 99 a[i] = b[i] + c[i] END DO</pre>

- Distribution of loop iterations over all threads in a Team.
- Scheduling of the distribution can be influenced.
- Loops often account for most of a program's runtime!

Worksharing illustrated







The Barrier Construct

- **OpenMP** barrier (implicit or explicit)
 - Threads wait until all threads of the current *Team* have reached the barrier

C/C++ #pragma omp barrier

• All worksharing constructs contain an implicit barrier at the end



The Single Construct

C/C++	Fortran
<pre>#pragma omp single [clause] structured block</pre>	<pre>!\$omp single [clause] structured block</pre>
	!\$omp end single

- The single construct specifies that the enclosed structured block is executed by only on thread of the team.
 - It is up to the runtime which thread that is.
- Useful for:
 - I/O
 - Memory allocation and deallocation, etc. (in general: setup work)
 - Implementation of the single-creator parallel-executor pattern as we will see later...



The Master Construct (will be deprecated in OpenMP 6.0)

C/C++	Fortran
<pre>#pragma omp master[clause] structured block</pre>	<pre>!\$omp master[clause] structured block !\$omp end master</pre>

- The master construct specifies that the enclosed structured block is executed only by the master thread of a team.
 - Replacement: see the masked construct later
- Note: The masked construct is no worksharing construct and does not contain an implicit barrier at the end.

Demo



Vector Addition



- *for*-construct: OpenMP allows to influence how the iterations are scheduled among the threads of the team, via the *schedule* clause:
 - schedule(static [, chunk]): Iteration space divided into blocks of chunk size, blocks are assigned to threads in a round-robin fashion. If chunk is not specified: #threads blocks.
 - schedule(dynamic [, chunk]): Iteration space divided into blocks of chunk (not specified: 1) size,
 blocks are scheduled to threads in the order in which threads finish previous blocks.
 - schedule(guided [, chunk]): Similar to dynamic, but block size starts with implementation-defined value, then is decreased exponentially down to chunk.
- **Default is** schedule (static).



Static Schedule

- > schedule(static [, chunk])
- \rightarrow Decomposition

depending on chunksize

→ Equal parts of size 'chunksize' distributed in round-robin

fashion







Static Schedule

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Pros?







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→ No/low runtime overhead







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Static Schedule

- > schedule(static [, chunk])
- \rightarrow Decomposition

depending on chunksize

→ Equal parts of size 'chunksize' distributed in round-robin fashion

Pros?

→ No/low runtime overhead

Cons?

→ No dynamic workload balancing







- Dynamic schedule
 - schedule(dynamic [, chunk])
 - Iteration space divided into blocks of chunk size
 - Threads request a new block after finishing the previous one
 - Default chunk size is 1



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- Dynamic schedule
 - schedule(dynamic [, chunk])
 - Iteration space divided into blocks of chunk size
 - Threads request a new block after finishing the previous one
 - Default chunk size is 1
- Pros ?
 - Workload distribution
- Cons?
 - Runtime Overhead
 - Chunk size essential for performance
 - No NUMA optimizations possible



Synchronization Overview

- Can all loops be parallelized with for-constructs? No!
 - Simple test: If the results differ when the code is executed backwards, the loop iterations are not independent. BUT: This test alone is not sufficient:

```
C/C++
int i, int s = 0;
#pragma omp parallel for
for (i = 0; i < 100; i++)
{
    s = s + a[i];
}</pre>
```

• *Data Race*: If between two synchronization points at least one thread writes to a memory location from which at least one other thread reads, the result is not deterministic (race condition).



Synchronization: Critical Region

• A Critical Region is executed by all threads, but by only one thread simultaneously (Mutual Exclusion).

C/C++
#pragma omp critical (name)
{
 ... structured block ...
}

• Do you think this solution scales well?





Programming OpenMP

Scoping

Christian Terboven

Michael Klemm





Scoping Rules

- Managing the Data Environment is the challenge of OpenMP.
- *Scoping* in OpenMP: Dividing variables in *shared* and *private*:
 - *private*-list and *shared*-list on Parallel Region
 - private-list and shared-list on Worksharing constructs
 - General default is *shared* for Parallel Region, *firstprivate* for Tasks.
 - Loop control variables on *for*-constructs are *private*
 - Non-static variables local to Parallel Regions are *private*
 - *private*: A new uninitialized instance is created for the task or each thread executing the construct
 - *firstprivate*: Initialization with the value before encountering the construct
 - *lastprivate*: Value of last loop iteration is written back to the initial thread
 - Static variables are *shared*

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OpenMP

Privatization of Global/Static Variables

- Global / static variables can be privatized with the *threadprivate* directive
 - One instance is created for each thread
 - Before the first parallel region is encountered
 - Instance exists until the program ends
 - Does not work (well) with nested Parallel Region
 - Based on thread-local storage (TLS)
 - TIsAlloc (Win32-Threads), pthread_key_create (Posix-Threads), keyword ____thread (GNU extension)

C/C++	Fortran
<pre>static int i; #pragma omp threadprivate(i)</pre>	SAVE INTEGER :: i !\$omp threadprivate(i)

Privatization of Global/Static Variables

- Global / static variables can be privatized with the *threadprivate* directive ullet

 - Based on thread-local storage (TLS)



Back to our example

C/C++

```
int i, s = 0;
#pragma omp parallel for
for (i = 0; i < 100; i++)
{
    #pragma omp critical
        { s = s + a[i]; }
}
```

It's your turn: Make It Scale!

OpenMP.



#pragma omp parallel

#pragma omp for
 for (i = 0; i < 99; i++)
 {
 s = s + a[i];</pre>

} // end parallel

}

(done)



do i = 0, 24

end do

 $S = S + S_1$

end do

 $s = s + s_{2}$

do i = 25, 49

 $s_1 = s_1 + a(i)$

 $s_{2} = s_{2} + a(i)$



end do do i = 50, 74 $s_3 = s_3 + a(i)$ end do $s = s + s_3$ do i = 75, 99 $s_4 = s_4 + a(i)$ end do $s = s + s_4$

do i = 0, 99

s = s + a(i)

The Reduction Clause

- In a *reduction*-operation the operator is applied to all variables in the list. The variables have to be *shared*.
 - reduction(operator:list)
 - The result is provided in the associated reduction variable

C/C++
int i, s = 0;
#pragma omp parallel for reduction(+:s)
for(i = 0; i < 99; i++)
{
 s = s + a[i];
}</pre>

Possible reduction operators with initialization value:

+ (0), * (1), - (0), & (~0), | (0), && (1), || (0), ^ (0), min (largest number), max (least number)

Remark: OpenMP also supports user-defined reductions (not covered here)

Example: Pi (1/2)

```
double f(double x)
{
    return (4.0 / (1.0 + x*x));
}
double CalcPi (int n)
{
    const double fH = 1.0 / (double) n;
    double fSum = 0.0;
    double fX;
    int i;
#pragma omp parallel for
```

```
for (i = 0; i < n; i++)
{
    fX = fH * ((double)i + 0.5);
    fSum += f(fX);
}
return fH * fSum;
}</pre>
```


Example: Pi (2/2)

```
double f(double x)
{
    return (4.0 / (1.0 + x*x));
}
```

```
double CalcPi (int n)
```

```
const double fH = 1.0 / (double) n;
double fSum = 0.0;
double fX;
int i;
```

```
#pragma omp parallel for private(fX,i) reduction(+:fSum)
    for (i = 0; i < n; i++)
    {
        fX = fH * ((double)i + 0.5);
        fSum += f(fX);
    }
    return fH * fSum;
}</pre>
```


Programming OpenMP

OpenMP Tasking Introduction

Christian Terboven Michael Klemm

Tasking Execution Model

Supports unstructured parallelism
 unbounded loops

<pre>while (<expr>) {</expr></pre>
}

```
void myfunc( <args> )
{
    ...; myfunc( <newargs> ); ...;
}
```

- Several scenarios are possible:
 - → single creator, multiple creators, nested tasks (tasks & WS)
- All threads in the team are candidates to execute tasks

Example (unstructured parallelism)

What is a Task in OpenMP?

- Tasks are work units whose execution
 may be deferred or...
 - \rightarrow ... can be executed immediately
- Tasks are composed of
 - → code to execute, a data environment (initialized at creation time), internal control variables (ICVs)
- Tasks are created...
 - ... when reaching a parallel region \rightarrow implicit tasks are created (per thread)
 - ... when encountering a task construct \rightarrow explicit task is created
 - ... when encountering a taskloop construct \rightarrow explicit tasks per chunk are created
 - ... when encountering a target construct \rightarrow target task is created

OpenMP Tasking Idiom

- OpenMP programmers need a specific idiom to kick off task-parallel execution: parallel masked
 - → OpenMP version 5.0 introduced the parallel master construct
 - → With OpenMP version 5.1 this becomes parallel masked

```
int main(int argc, char* argv[])
 1
 2
    {
 3
         [...]
        #pragma omp parallel
 4
 5
 6
           #pragma omp masked
 7
 9
start task parallel execution();
 9
10
11.
         [...]
12.}
```

```
int main(int argc, char* argv[])
 1
 2
    {
 3
         [...]
        #pragma omp parallel
 4
 5
           #pragma omp single
 6
 7
 9
start task parallel execution();
 9
10
11.
         [...]
12.}
```


Fibonacci Numbers (in a Stupid Way ⁽²⁾)

<pre>int main(int argc,</pre>	14 int fib(int n) {
<pre>char* argv[])</pre>	15 if $(n < 2)$ return n;
{	16 int x, y;
[]	17 #pragma omp task shared(x)
<pre>#pragma omp parallel</pre>	18 {
{	19 $x = fib(n - 1);$
<pre>#pragma omp masked</pre>	20 }
{	21 #pragma omp task shared(y)
fib(input);	22 {
}	23 $y = fib(n - 2);$
}	24 }
[]	25 #pragma omp taskwait
. }	26 return x+y;
	27.}

- Only one thread enters fib() from main().
- That thread creates the two initial work tasks and starts the parallel recursion.
- The taskwait construct is required to wait for the result for x and y before the task can sum up.

13.

T1 enters fib(4)

Task Queue

- T1 enters fib(4)
- T1 creates tasks for fib(3) and fib(2)

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- T1 and T2 create 4 new tasks

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- • •

Programming OpenMP

Hands-on Exercises

Christian Terboven Michael Klemm

Exercises

- We have implemented a series of small hands-on examples that you can use and play with.
 - Download: https://github.com/NERSC/openmp-series-2024
 - → Build: make

- Each hands-on exercise has a folder "solution"
 - \rightarrow It shows the OpenMP solution that we have added
 - \rightarrow You can use it to cheat \odot , or to check if you came up with the same solution

Exercises: Overview

Exercise no.	Exercise name	OpenMP Topic	Day / Order (proposal)
1	Hello World	Getting started	Start with this (if OpenMP is new for you)
2	Pi	Worksharing, Scoping	First day
3	Jacobi	Worksharing, Scoping	First day
4	Work-Distribution	Worksharing	First day
5	Min/Max	Worksharing, Reduction	First day

to be continued ...